Non-Fermi-liquid behavior and superconducting fluctuations caused by hybridization

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The exact solution is proposed that describes the low-energy properties of conduction electrons hybridized with localized $5f$ electrons. For small concentrations of the latter, the solution for $5f$ orbitals manifests a mixed valence and crossover from a Fermi-liquid-like behavior at very low energies to the two-channel non-Fermi-liquid behavior at higher energies. For the finite concentration of localized electrons the same hybridization dynamically yields an attraction between conduction electrons, resulting in superconducting fluctuations (Cooper-like pairs) present in the low-temperature phase. We predict a quantum transition to the phase, in which superconducting fluctuations coexist with magnetic ones. Possible relevance of our results to the data of experiments in some U-based compounds is discussed.

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I. INTRODUCTION

There has recently been a renewed interest in heavy-fermion systems. While the nature of many effects for lanthanide-based heavy-fermion systems is understood, the one for actinides often remains to be clarified. As an example, one can consider the non-Fermi-liquid (NFL) behavior of the normal phases, superconductivity, and coexistence of the latter with magnetic fluctuations in certain U-based heavy-fermion compounds.[1,2] Here, we propose an exactly solvable model to describe some of the important effects caused by the hybridization of $5f$ electrons of U ions with conduction electrons. Our exact solution reveals several remarkable properties. For a small concentration of $5f$ orbitals the critical NFL behavior persists, while the hybridization with the finite concentration of localization orbitals dynamically induces the creation of Cooper-like pairs and a spin gap of unbound conduction electrons. As the concentration increases for strong quasidegeneracy of the mixed configurations of the $5f$ orbitals, the gap closes, signaling a quantum phase transition to an uncompensated ferrimagnetic phase (coexisting with superconducting fluctuations). To the best of our knowledge, this is the first exact study where the hybridization between two almost degenerate configurations of $5f$ orbitals and conduction electrons produce *both* NFL physics in the dilute limit of U ions and superconducting fluctuations of conduction electrons in the dense limit of U ions. Notice that there is *no direct interaction* between conduction electrons, so that the pairing between them exists only because of the hybridization between them and localized $5f$ electrons. It turns out that a fully nonperturbative analysis of the relevant physics of *both* situations is allowed from the grounds of *the same* model.

It is usually accepted that magnetic properties of U ions are determined by $5f$ orbitals [in real materials it pertains to the configurations $5f^2$ of U^{4+} ion or $5f^3$ (U^{3+})]. Some U compounds manifest two almost degenerate low-energy states of the $5f$ configurations of U ions: the $5f^3$ of U^{3+} and $5f^2$ of U^{4+};[3] the mixed valence behavior of U ions results. Let us classify possible electron-electron interactions in metallic compounds with $5f$ orbitals. The Coulomb interaction of $5f$ electrons of the same orbital (which we enumerate with index j) can be described by the Hamiltonian $\mathcal{H}_C^j = \Sigma_{mm',\sigma\sigma'} U_{m,m'} f^\dagger_{j,m,\sigma} f_{j,m,\sigma} f^\dagger_{j,m',\sigma'} f_{j,m',\sigma'}$. Here $U_{m,m'}$ is the Coulomb constant, and $f^\dagger_{j,m,\sigma}$ creates an electron at the f orbital (at site x_j) with the projection of the orbital moment m and spin $\sigma = \pm\frac{1}{2}$. It is the strongest interaction between electrons in $5f$ orbitals.[4] Note though that the Coulomb repulsion in actinides is estimated to be smaller than for rare-earth ions since $5f$ wave functions are more extended than $4f$ wave functions. In what follows we shall use the fact that $U_{m,m'}$ is large enough, so that *multiple electron occupations of orbital states will be excluded*. The next leading term in the (local) Hamiltonian of $5f$ electrons is the Hund's *exchange* coupling. Its Hamiltonian has the form

$$\mathcal{H}_H^j = \sum_{mm',\sigma\sigma'} J_{H,m} f^\dagger_{j,m,\sigma} f_{j,m',\sigma} f^\dagger_{j,m',\sigma'} f_{j,m,\sigma'}, \qquad (1)$$

with $J_{H,m} > 0$. Although spin-orbit coupling is relatively large for heavy atoms like U, it was found to be of minor importance compared with Hund's coupling.[4] A crystalline electric field in U compounds deforms the degenerate $5f$ orbitals and brings an anisotropy to the hybridizations between deformed orbitals and conduction electrons. This differs from the usual role of the crystalline electric field in lanthanide compounds like Ce-based rare-earth systems. One group of the localized U electrons hybridizes more strongly with ligands and are almost completely delocalized, while the hybridization of others with ligands is smaller and they are mostly localized. Hence the hybridization Hamiltonian can be written as

$$\mathcal{H}_{hyb}^j = \sum_{m\sigma,\tau} \delta(x - x_j) V_m a^\dagger_{m,\sigma}(x) |j\,0\,m\rangle\langle j\,S\,\tau\,m| + \text{H.c.}, \qquad (2)$$

where $a^\dagger_{m,\sigma}(x)$ are creation operators for conduction electrons and the bra and kets denote the states of the localized electrons in $5f$ orbitals, with spin S, its projection τ, and

orbital index m (the energy of the delocalized orbitals is higher than the localized one[4]). The dependence of the hybridization element V_m on m manifests possible anisotropy in hybridization with conduction electrons. The Hamiltonian of conduction electrons can be presented in the long-wave form

$$\mathcal{H}_{cond}=-\sum_{m,\sigma}\int dx a^{\dagger}_{m\sigma}(x)\times\{i\partial_x+(1/\Lambda)\times[\partial_x^2-V(x)]\}a_{m\sigma}(x), \tag{3}$$

where

$$V(x)=\sum_{j}^{N_i}\delta(x-x_j)(x/|x|)[\delta'(x+0)+\delta'(x-0)].$$

The counterterm [with $V(x)$] is necessary to preserve the integrability at the positions x_j of N_i $5f$ orbitals. The parameter Λ measures the curvarture scale of the spectrum.[5] The inclusion of the counterterm does not principally affect physical properties of a single hybridization impurity (cf. Ref. 5). As for the dense limit, we emphasize that the sign of the counterterm is *positive*, so that it cannot produce an attraction between conduction electrons. Pairs (see below) cannot be created due to that term. It is known that the wave function of $5f$ electrons of U ions are more extended than $4f$ electrons of rare-earth ions.[2] That is why one usually has to take into account a possible direct interaction of electrons between $5f$ orbitals of neighboring U ions. Most often it is considered as a magnetic Ruderman-Kittel-Kasuya-Yosida (RKKY) interaction through conduction electrons. To model a RKKY interaction between the localized electrons of different sites in real U compounds, we add a direct hopping of $5f$ electrons between neighboring U ions with the Hamiltonian $\mathcal{H}_{hop}=-\Sigma_{j,j',m,\sigma}(f^{\dagger}_{j,m,\sigma}f_{j',m,\sigma}+\text{H.c})$. [The integral of such a hopping is much less than the intershell $5f$ electron-electron interaction ($U_{m,m'}$,$J_{H,m}$); hence, in the first nonzero approximation, it produces a direct exchange coupling between the spins of localized electrons.] We shall consider that hopping in the long-wave limit, too. In this way the total studied Hamiltonian is $\mathcal{H}=\Sigma_j[\mathcal{H}^j_H+\mathcal{H}^j_{hyb}]+\mathcal{H}_{cond}+\mathcal{H}_{hop}$.

II. SCATTERING PROCESSES AND BETHE ANSATZ EQUATIONS

Let us first treat the simplified *orbital-isotropic* hybridization (i.e., $V_m=V$). We shall return to the effect of the hybridization anisotropy below. Three scattering processes are possible: (i) the scattering of conduction electrons off localized ones, (ii) the scattering between localized electrons, and (iii) the scattering between conduction electrons. The two-particle scattering matrix (TPSM) of the process (i) is diagonal in orbital sector, and in the spin subspace it has the form (with $\Lambda\gg 1$)

$$\hat{S}(k)=\frac{(k-\theta)\hat{I}_\sigma-ic\hat{P}_\sigma}{k-ic}, \tag{4}$$

where $c=V_m^2$, $\theta=\epsilon_{f^3}-\epsilon_{f^2}-\mu-\text{const}\geqslant 0$ (μ is the chemical potential and $\epsilon_{f^{2,3}}$ are the energies of the lowest levels of $5f^{2,3}$ configurations, respectively). $\hat{I}_\sigma$ and $\hat{P}_\sigma$ denote the identity and permutation operators in the spin subspace. Hence the lowest configuration of $5f^2$ orbital (with zero effective spin) can temporarily absorb the spin of one conduction electron to form an effective spin $S=\frac{1}{2}$, i.e., the $5f$ localized site is mixed valent and its wave function is a linear superposition of two different configurations. Each state of each of the localized electrons has to satisfy the completeness condition $\Sigma_{m,\tau}|S\tau m\rangle\langle S\tau m|+|0m\rangle\langle 0m|=1$. The TPSM for process (ii) factorizes into the one for the spin sector and the one for the orbital sector as

$$\hat{R}(k)=[k'\hat{I}_\sigma-ic'\hat{P}_\sigma]\times[k'\hat{I}_m+ic'\hat{P}_m]/[(k')^2+(c')^2], \tag{5}$$

where $k'=(k_1-k_2)/\Lambda$, $2c'=J_{H,m}$. $\hat{I}_m$ and $\hat{P}_m$ are the identity and permutation operators in the orbital subspace. Those matrices satisfy the Yang-Baxter relations (YBR) mutually and with $\hat{S}$ if $c=\Lambda c'$. YBR are the necessary and sufficient conditions for the integrability.[6,7] Hence the exact solvability of the model demands the restriction on the values of the hybridization elements $J_{H,m}=2V_m^2/\Lambda$. The TPSM between conduction electrons (iii) have to satisfy the YBR with $\hat{S}$ and $\hat{R}$ (and mutually) also to preserve the integrability. Formally, there is no direct coupling between conduction electrons in our model. However, the naive choice of the diagonal scattering matrices for the TPSM of process (iii) does not satisfy the YBR. The correlations between conduction electrons are *induced through the hybridization with localized electrons*. Hence the hybridization of conduction electrons with the (interacting) electrons in $5f$ orbitals *dynamically correlates* the motion of formers. That is why the TPSM between conduction electrons dynamically obtains the form of $\hat{R}(k)$. The two-electron wave function (WF) of conduction electrons can be written as a product of a coordinate WF, a spin WF, and an orbital WF. The WF has to be antisymmetric under the exchange of two particles. Hence, if the spin and orbital parts have the same symmetry, the coordinate WF is antisymmetric and vanishes if $x_1=x_2$ (with $x_{1,2}$ being the coordinates of the electrons), so that the electrons cannot interact. Conducting electrons then necessarily form a spin singlet and orbital triplet or a spin triplet and orbital singlet. The former corresponds to an attractive Hund's coupling ($J_{H,m}>0$), while for the latter that interaction is repulsive. When applied to a triplet (either in the spin or the orbital sector) WF, the corresponding TPSM yields one, while if it acts on a singlet it gives rise to a phase shift. For the case of spin and orbital singlets the two phase factors cancel, and there is no effective interaction between the conduction electrons. It is important to emphasize that the TPSM of conduction electrons dynamically obtains the form of $\hat{R}(k)$ even for $J_{H,m}=0$; i.e., it can be caused *only by the hybridization*, cf. Ref. 5.

In order to determine the spectrum and the eigenfunctions of our model, we impose periodic boundary conditions and solve the corresponding Schrödinger equations by means of

Bethe's ansatz. The procedure is standard and we skip the details. The energies and eigenstates of our model are parametrized by three sets of *rapidities*: charge rapidities $\{k_j\}_{j=1}^{N}$ (with N the number of electrons), spin rapidities $\{\lambda_\alpha\}_{\alpha=1}^{M}$ (with M the number of down spins), and orbital rapidities $\{\xi_\beta\}_{\beta=1}^{n}$ (with n the number of electrons in the $m=1$ orbital). In principle a crystalline electric field lifts the degeneracy of orbitals, the latter becoming unequally populated. Each eigenstate corresponds to a solution of the Bethe ansatz equations (BAE), here obtained on a periodic interval of length L (for simplicity we limit ourselves with only two orbital indices). For the hybridization-isotropic case with $c=V^2$, we get

$$e_1^{N_i}(\Lambda f_j-\theta')e^{ik_jL}=\prod_{\gamma=1}^{M} e_1(f_j-\lambda_\gamma)\prod_{q=1}^{n} g_1^{-1}(f_j-\xi_q),$$

$$\prod_{j=1}^{N} e_1(\lambda_\alpha-f_j)=-\prod_{\delta=1}^{M} e_2(\lambda_\alpha-\lambda_\delta),$$

$$\prod_{j=1}^{N} g_1(\xi_\beta-f_j)=-\prod_{\gamma=1}^{n} g_2(\xi_\beta-\xi_\gamma), \qquad (6)$$

where $f_j=k_j/c\Lambda$, $\theta'=\theta/c$, $e_n(y)=(2y-in)/(2y+in)$, $j=1,\ldots,N$, $\alpha=1,\ldots,M$, $\beta=1,\ldots,n$, and $g_n(y)=e_n(y)$. The energy is given by

$$E=\sum_{j=1}^{N}[c\Lambda f_j(1+cf_j)-2x\pi a_1(c\Lambda f_j-\theta)], \qquad (7)$$

where $a_n(y)$ is the Fourier transform of $\exp(-n|pc|/2)$. The last term (with $x=N_i/L$ being the concentration of $5f$ orbitals) is caused by the added direct antiferromagnetic interaction between $5f$ electrons. In the case when *all* electrons are localized the last term collapses to the well-known energy of a Heisenberg spin-exchange antiferromagnetic model. The fact that energies and eigenstates are blind to the spatial positions of orbitals is an artifact of integrability. However, real systems[8] often exhibit a large quasidegeneracy of the states as a function of the distribution of hybridization impurities for stoichiometric compounds. The BAE of our (hybridization-isotropic) model and those of Ref. 9 are similar. However, there is a drastic difference between the present study and previous approaches.[9,10] Namely, in previous studies the *internal interaction between conduction electrons* was the reason for the nontrivial scattering between conduction electrons. In contrast, in the present treatment, there is no *a priori* attraction between conduction electrons. The nontrivial scattering between conduction electrons is the *consequence of the hybridization* between them and $5f$ electrons. Notice also the difference in the structure of the BAE Eqs. (6) and those from Ref. 10. That difference originated from the different nature of studied hybridization. (In Ref. 10 the hybridization absorbs the spin of one conduction electron and forms a *smaller* effective spin $S'=S-\frac{1}{2}$ of the orbital, opposite to the present case and that of Ref. 9.) However, our system with the Hund's exchange of localized electrons and the hybridization of $5f$ electrons with conduction electrons behaves analogously to the system of *interacting* conduction electrons coupled to impurities.[9,10] It is not a surprise because the TPSM of these problems satify the YBE mutually.

The hybridization anisotropy (i.e., let $V_1 \leqslant V_2$) and the orbital-anisotropic exchange interaction between the localized electrons produces several important changes. [Notice that the effect of a crystalline electric (orbital) field results similar to the one of a hybridization anisotropy.[4,11]] When treating the hybridization anisotropic case for the TPSM, we proceed along the lines pioneered in Ref. 5. Then, following the standard procedure, we obtain the BAE and the expression for the eigenenergy. The BAE for the hybridization-anisotropic situation in the scaling regime formally get similar form as Eqs. (6), but with $c_j=V_j^2$ and $g_n(y)=\sinh\nu(y-in/2)/\sinh\nu(y+in/2)$ (ν characterizes the anisotropy, cf. Ref. 5)

$$e_1^{N_i}(\Lambda f_j-c_j^{-1}-\theta')e^{ik_jL}=\prod_{\gamma=1}^{M} e_1(f_j+c_j^{-1}-\lambda_\gamma)\times\prod_{q=1}^{n} g_1^{-1}(c_1f_jc_j^{-1}-\xi_q),$$

$$\prod_{j=1}^{N} e_1(\lambda_\alpha-f_j-c_j^{-1})=-\prod_{\delta=1}^{M} e_2(\lambda_\alpha-\lambda_\delta),$$

$$\prod_{j=1}^{N} g_1(\xi_\beta-c_1f_jc_j^{-1})=-\prod_{\gamma=1}^{n} g_2(\xi_\beta-\xi_\gamma), \qquad (8)$$

where $j=1,\ldots,N$, $\alpha=1,\ldots,M$, $\beta=1,\ldots,n$, ($c_j=V_j^2$). For the anisotropic hybridization we renormalize $a_n(y)$ to $a_n^j(y)$, the Fourier transform of $\exp(-n|pc_j|/2|)$.

III. LOW-ENERGY PROPERTIES

The main features of the low-energy behavior of our model are determined by its ground state. It is obtained by filling up the Dirac seas of low-lying excitations, i.e., by populating all possible eigenstates with negative energies. We can divide our study into two important cases: the low concentration of $5f$ orbitals and the *finite* concentration of them, $x\neq 0$. In the former case in the thermodynamic limit $x\to 0$, i.e., localized electrons behave as *single* impurities. For the latter case correlation effects between localized electrons have to be taken into account.

For $N_i=1$, we put $\Lambda\to\infty$ in Eqs. (6)–(8).[5] This means that Λ increases with the decrease of the concentration of $5f$ orbitals. The standard way to find the solution to Eqs. (6) or (8) is the *fusion* procedure.[6] It is the search of a solution to BAE for charge rapidities within the class of *strings* (orbital-singlet bound states) of the complex form $f_q=c_1c_j^{-1}(\xi_q\pm i\frac{1}{2})$ ($j=1,2$).[5] Those of them that have maximal spin are only important for the low-energy physics.[6] The length of those strings is determined by the number of orbitals (channels), i.e., for our case, it is 2. One conduction electron,

however, is bound at the $5f$ orbital (i.e., we have its charge rapidity real $k_q=\theta$ with the fixed ratio θ/Λ). In the limit of $\Lambda\to\infty$ all real parts of those string solutions can be neglected[5] (except for the rapidity of the conduction electron bound at the $5f$ orbital). An additional meaning of the fusion is the filling of all interorbital bound-state solutions to BAE. In fact, the fusion is a way of eliminating orbital (channel) rapidities from BAE. After that procedure spin rapidities become present in the fused BAE only as $\lambda_\gamma - c_j^{-1}\pm(1\pm\phi_j)$, where $\phi_j=c_1/c_j$ $(j=1,2)$. Hence the hybridization anisotropy yields (via the filling of inter-orbital bound states) four kinds of low-lying bulk spin excitations, which have Dirac seas: spinons (spin strings of length 1 or real spin rapidities), spin strings of length 2, and spin composites with the effective lengths $(1\pm c_1/c_2)$. In the isotropic limit $c_1=c_2$, we recover the only bound states of length 2 relevant in the low-energy physics of the system, which is characteristic of the two-channel Kondo problem. In the opposite case of vanishing V_1 or V_2, i.e., when the localized electrons with only one orbital index hybridize with conduction electrons, we recover the standard single-channel Kondo case. For the behavior of the hybridization impurity (the conduction electron bound at the $5f$ orbital) two low-energy scales are important: $T_K=(N/L)\exp[-\pi(\theta+1)c_1^{-1}]$ and $T_a=(N/L)\cos(\pi c_1/2c_2)\exp[-\pi(\theta+1)c_2^{-1}]$. One can see that the parameter θ also measures the exchange coupling of the localized effective spin to the spins of conduction electrons $\mathcal{J}\sim\theta^{-1}$. The antiferromagnetic effective exchange between the spins of neighboring $5f$ orbitals in our model is proportional to $\Lambda^{-2}\sim\theta^{-2}$. This is consistent with the standard condition for a RKKY interaction, which is proportional to $\mathcal{J}^2$.

The solution of BAE reveals that in the ground state (for small enough θ) the mixed valence of the $5f$ orbital increases with growing the band filling of conduction electrons from 2 $(5f^2)$ for the empty band to 3 $(5f^3)$. (It means that the valence of the $5f$ orbital explicitly depends on the *total number of electrons* in the system.) The ground-state magnetization of the localized electron for $H\ll T_a\ll T_K$ (H is an external magnetic field) is proportional to H/T_a with the standard Kondo logarithmic corrections, i.e., $M^z_{loc}\sim H/T_a(1+|\ln H/aT_a|^{-1}-\cdots)$ (a is some nonuniversal constant). The latter are characteristic to the asymptotically free behavior of an impurity spin. It is usual for a simple one-channel Kondo problem[6] with a finite magnetic susceptibility. However, for $T_a\ll H\ll T_K$, the magnetization of the $5f$ orbital reveals the logarithmic behavior $M^z_{loc}\sim-(H/T_a)\ln(H/aT_K)$ (with divergent susceptibility), typical for the two-channel Kondo behavior. For $T\ll T_a\ll T_K$, we obtain the low-T (Sommerfeld) coefficient of the specific heat for the localized electron

$$\gamma_{loc}\sim T_a^{-1}[1-(3T_a\pi T_K)\ln(T_a/T_K)](1+|\ln T/T_a|^{-1}-\cdots)$$

and the finite ground-state susceptibility

$$\chi_{loc}\sim T_K^{-1}\ln(T_a/T_K)(1+|\ln T/T_K|^{-1}-\cdots)$$

(both with usual logarithmic corrections of an asymptotically free spin). This case pertains to the single-channel Kondo physics, although two different energy scales for χ_{loc} and γ_{loc} mean that the Wilson ratio differs from the FL one. For $T_a\ll T\ll T_K$ we have $\gamma_{loc}\propto\chi_{loc}\sim-(T_K)^{-1}\ln(T/T_K)$ (i.e., logarithmically divergent) and with the remnant entropy of the $5f$ orbital $\mathcal{S}_{loc}=\ln\sqrt{2}$. For higher temperatures the magnetic susceptibility of the $5f$ orbital manifests the Curie-like behavior with usual logarithmic corrections. The temperature dependence of the (magneto)resistivity is determined by the scattering of conduction electrons off the spins of localized electrons (magnetic impurities). We calculate it in a standard way, taking into account subleading irrelevant perturbations.[2] It can be approximated (for a small hybridization anisotropy) at low temperatures by

$$\rho(T)\sim\rho_0-A(T/T_a)^2(1+|\ln T/T_a|^{-1}-\cdots)$$

for $T\ll T_a\ll T_K$ and

$$\rho(T)\sim\rho_0'+B(T/T_K)^{1/2}(1+|\ln T/T_K|^{-1}-\cdots)$$

for $T_a\ll T\ll T_K$ (also with logarithmic corrections of the asymptotically free spin of the impurity).[6]

IV. FINITE CONCENTRATION

Now we turn to the case of the finite concentration of $5f$ orbitals. Hence we keep $x\neq0$ and Λ finite. Absolutely analogous to Ref. 9 we can show that only (gapped) unbound conduction electrons, Cooper-like pairs (spin-singlet orbital-triplet charged bound states of electrons) and interorbital bound states of conduction electrons (orbital strings of lengths 1 and 2) have negative energies. Thus only those low-lying excitations make up the Dirac seas defining the ground state of the model. This means that all the states with negative energies are filled in the ground state, while others are empty. Noninteracting (see below) spin-singlet pairs have bosonic symmetric wave functions. However, they are hard-core bosons, this is why they have their Dirac sea too. These Cooper-like pairs persist at any temperature, but since the movement of electrons is effectively one dimensional (1D) in our model, there is no global phase coherence between pairs, and hence no long-range order. However, the pairing implies a critical field H_{c1} (equal to the gap of unbound conduction electron excitations) at zero temperature, below which there is no magnetic response, reminiscent of the Meissner effect. Naturally, there exists an additional critical field, H_{c2}, at which all the spins of the system become aligned parallel to the magnetic field. All pairs are absent in this domain of fields, and unbound electron excitations are gapped. A small coupling between 1D subsystems, though, usually can produce a long-range superconducting ordering with pairs existing only in the low-temperature phase. Note that magnetic impurities in BCS superconductors break the time-reversal symmetry and act as Cooper pair breakers,[12] thus reducing the critical temperature and the gap. The gap can be closed before the superconductivity is destroyed—an effect that is known as gapless superconductivity. In our model, in contrast to the standard BCS-like approach, the finite concentration of (magnetic) $5f$ electrons, on the one hand, *causes* an attraction between conduction electrons

through the hybridization and tends to enhance the density of states of Cooper-like pairs. On the other hand, the same $5f$ orbitals act as magnetic impurities and tend to destroy superconducting fluctuations. The total effect, as will be shown below, strongly depends on the value of θ (the difference between the energies of the lowest nonmagnetic and magnetic configurations of the $5f$ orbitals, or, in other words, off-resonance shifts for single impurities).

The introduction of a finite concentration $x \neq 0$ of $5f$ orbitals drastically affects the ground state (and, in fact, all states that are effectively present at $T \ll H$, in the case that an external magnetic field is applied). To see how this comes about, we study the integral equations for the ''dressed'' (due to interactions) energies of low-lying excitations. In the case of zero total orbital moment, this can be done analytically, similar to, e.g., Refs. 9 and 10. For zero total orbital moment the interorbital bound states can be eliminated. Then the integral equations for the dressed energies for unbound electron excitations (ε) and Cooper-like pairs (Ψ) at $H=0$ have the form

$$[2-G_1-G_{c_1/c_2}]\circ\varepsilon+[2G_0-G_2+G_{c_1/c_2}]\circ\Psi = 2\varepsilon_0(k)-2\mu-2\pi x\sum_{j=1,2} a_1^j(k-\theta),$$

$$[2G_0-G_2+G_{c_1/c_2}]\circ\varepsilon-2\Psi_0(\lambda)+2\pi x\sum_{j=1,2} a_2^j(\lambda-\theta)bf = [2+G_1+G_3-G_{c_1/c_2}-G_{3c_1/c_2}]\circ\Psi-4\mu, \quad (9)$$

where $\circ$ denotes convolution over the Dirac seas[9] and

$$2\Lambda\varepsilon_0(k)=(4k+\Lambda)^2-\frac{1}{2}\Lambda^2 \ ,$$

$$2\Lambda\Psi_0(\lambda)=2(4\lambda+\Lambda)^2-\Lambda^2. \quad (10)$$

The kernels are determined from the formula

$$G_a(x)=\frac{1}{2\pi}\int du\,\frac{\exp(-iux-a|uc_2|/2)}{2\cosh(c_2u/2)}. \quad (11)$$

It is important to emphasize that the antiferromagnetic exchange between neighboring $5f$ orbitals *does not* produce additional Dirac sea for pure spin excitations in this model, which is clear from the analysis of Eqs. (9). This differs from the situation in Refs. 9 and 10.

The value of the spin gap Δ is one-half of the smallest energy required to overcome the binding energy and to unpair the Cooper-like spin-singlet state. (On the other hand, the value of the spin gap coincides with H_{c1}.) The value of the gap depends on the concentration of $5f$ orbitals. In the orbital-isotropic hybridization (and $H=0$), we find

$$\Delta=[\Psi_0(Q)+2\pi x a_2(Q-\theta)][\tfrac{1}{2}-G_0]-2\pi x a_1(\theta) - G_0\circ[\Psi_0(\lambda)-2\pi x a_2(\lambda-\theta)], \quad (12)$$

where the integration is over the Dirac sea for pairs with Q denoting their Fermi points. In the trivial limit $V_m \to 0$, the gap vanishes since there is no binding between conduction electrons (all the TPSM in this case are unities). Notice that the terms proportional to the concentration x appear due to the inclusion of the direct transfer of electrons between $5f$ orbitals at neighboring sites (antiferromagnetic exchange between $5f$ neighboring orbitals). The degree of degeneracy of $5f$ orbitals at the same site (i.e., the difference between the energies of the lowest magnetic $5f^3$ and nonmagnetic $5f^2$ configurations of $5f$ orbitals, θ) determines whether the spin gap becomes smaller or larger with the increase of concentration of $5f$ orbitals. For large θ the gap of unbound conduction electron excitations *increases* if the number of paired electrons is large due to an enhancement of the density of states of pairs. In contrast, for small θ the spin gap *decreases* with increasing x and *closes* at the critical concentration x_c. Thus the gap of low-lying unbound conduction electron excitations decreases for almost degenerate lowest states of $5f^2$ and $5f^3$ configurations of U ions. On the other hand, when the difference between the lowest energies of those magnetic and nonmagnetic configurations becomes large, the gap increases linearly with the number of $5f$ orbitals, hence with the enhancement of the superconductiving fluctuations. In fact, such a behavior is the consequence of the presence of antiferromagnetic correlations between the neighboring $5f$ orbitals. The parameter θ itself can depend on x, consistent with the experimental situation Ref. 2 (or if one takes into account that the Fermi points of pairs Q are slightly x dependent, which manifests the conservation of the total number of electrons), yielding the *nonlinear* in the concentration x effect.

There are no additional unbound electron excitations appearing when the gap is open (i.e., for $x<x_c$). Hence, the presence of localized (magnetic) $5f$ electrons *does not lead to a pair breaking* of conduction electrons for such concentrations, in contrast to the suppression of a superconductivity in ordinary BCS-like superconductors.[12] The charge and magnetic subsystems are effectively *disconnected* for $x<x_c$. In this phase magnetic $5f$ electrons are antiferromagnetically compensated, which coexists with superconducting fluctuations of Cooper-like spin-singlet pairs. However, the gap may become negative when $x>x_c$. Thus, unbound conduction electron excitations (with $k_F \sim \sqrt{x-x_c}$) appear to have their Dirac sea (i.e., for some of them their energies become negative) *in the absence of a magnetic field*, signaling a *quantum phase transition* to a ferrimagnetic phase (with a weak magnetic moment). It is the quantum phase transition, because it is governed by the change of concentration of $5f$ orbitals, not of the temperature as for usual phase transitions. Cooper-like pairs are still present for $x>x_c$, reminiscent of type-II superconductivity.[12] In this phase the weak magnetism (ferrimagnetism) coexists with superconducting fluctuations. For nonzero H smaller than the critical field $H_{c1}(x)$, the spin gap persists for $x<x_c$, and there are no unbound electrons in the system. The critical field $H_{c1}(x)$ decreases with increasing concentration x and vanishes when x approaches x_c. The critical line separating the gapless and gapped (ferrimagnetic) phases manifests itself in the van Hove singularity of the opening of the band of

unbound electron excitations. The critical behavior at the quantum phase transition point $x=x_c$, $H=0$ is also revealed in the scaling dimensions: the dressed charge matrix[7] gets enlarged from 3×3 to 4×4 with the additional off-diagonal components proportional to $\sqrt{x-x_c}$. The band of pairs produces a nonzero coefficient for the low-T specific heat ($\sim T$ in one dimension). In contrast, at the critical lines, the van Hove singularities of empty bands produce a $\sqrt{T}$ behavior of the specific heat.

The above-mentioned effect persists for $c_1\neq c_2$. For that case, however, the hybridization anisotropy causes the effective interaction between pairs (they become not free as in the previous case). For a small hybridization anisotropy $|V_1-V_2|\ll V_2$, the scaling dimension of pairs in our effectively 1D model is $1-o((V_1-V_2)^2/V_2^2)$. Pairs are *almost free* hard-core bosons for a small nonzero anisotropy. The standard 3D coupling between effective 1D subsystems yields the power-law low-T behavior of the specific heat (for $T<T_c$) with the exponent $3-o((V_1-V_2)^2/V_2^2)$. The deviation of the exponent from 3 is as larger, as larger the anisotropy of the hybridization of conduction electrons with the ones of $5f$ orbitals.

V. DISCUSSION AND CONCLUSIONS

Let us briefly discuss the possible relevance of our results for real systems. The effective one dimensionality of our model for large concentrations of $5f$ orbitals introduces features not seen in higher dimensions. However, even a small coupling between 1D subsystems results in the phase transition for low T to the ordered superconducting state. Such a weak coupling determines the small critical temperature, which is consistent with observations for U-based heavy-fermion superconductors.[2] (Note, though, that the presence of possible nodes on the Fermi surface of conduction electrons in two or three dimensions or electron-phonon coupling may change the picture.) It turns out that our (even simplified) model shares a number of important characteristics with some real U-based heavy-fermion compounds, e.g., alloys $U_xTh_{1-x}Be_{13}$. Among them, we can point out a huge enhancement of the effective mass of carriers in the normal phase of those U alloys;[13] the mixed valence of localized $5f$ electrons there;[3] the critical NFL behavior in the normal (nongapped) low-temperature phase [of the low-temperature spin susceptiblitity $\chi\sim\chi_0-\sqrt{T}$, specific heat $C\sim -T\ln T$ and (magneto)resistivity $\rho\sim\rho_0+B\sqrt{T}$ with a crossover at 2 K];[2] the power-law behavior ($\sim T^3$) of the low-T specific heat in the presence of a spin gap;[13] the scattering of conduction electrons off two configurations of U ions;[3] a phase with a weak ferromagnetic moment for a certain range of concentrations of U;[14] and the coexistence of superconducting and magnetic fluctuations for some concentrations of U ions[1] and (quantum) phase transitions driven by a change of the concentration of U ions.[1,14]

To summarize, in this paper we have exactly studied the effects of a hybridization between the mixed configurations of $5f^2$ and $5f^3$ orbitals and conduction electrons. A finite fraction of the electrons is localized, producing a mixed valence of $5f$ orbitals. For small concentration of $5f$ orbitals a hybridization anisotropy yields two low-energy scales with the critical NFL behavior of the localized electrons. For a finite concentration of orbitals the hybridization dynamically induces an attraction between conduction electrons, which results in the creation of Cooper-like pairs and the spin gap for unbound electron excitations. This important result was obtained by an exact method taking *all* possible fluctuations into account, with no *a priori* assumption of a (local) symmetry breaking. Note that an attraction between conduction electrons due to the hybridization (hence a large effective mass) implies a short coherence length $\xi_0\propto\pi v_F/\Delta$, consistent with the relatively short coherence lengths in U-based superconductors. The main criticism of our previous studies[10] was connected with the fact that in the previous model superconducting fluctuations were caused by the *initial* interaction between the conducting electrons (i.e., they were *not* caused by the interaction of conduction electrons with $5f$ electrons). In the present model the critical NFL behavior of the system for the small concentration of the localized electrons and superconducting correlations for large concentrations of the latter are the *consequences of the same hybridization with* $5f$ *electrons*. We predict that the spin gap may be closed for concentrations of $5f$ orbitals above some critical value, at which unbound electron excitations appear. Emergence of that effect depends on the degree of the quasidegeneracy between the lowest levels of $5f^2$ and $5f^3$ configurations of $5f$ orbitals. The total magnetization of the system *spontaneously* becomes nonzero (for $H=0$), implying a quantum phase transition (governed by the change of concentration of $5f$ orbitals) to a *ferrimagnetic* phase with coexisting superconducting fluctuations (pairs). Naturally, our simplified model cannot explain *all* the features of real alloys. However, any of existing models of $U_xTh_{1-x}Be_{13}$ (see, e.g., Ref. 2) cannot exactly manifest a non-Fermi-liquid behavior of the normal phase and phases with coexistence of superconducting and magnetic fluctuations in low-temperature phases.

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